Thioacetamide

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 6.43 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.18e-01

Confidence level: 6.80e-01

Nearest Neighbors from the Training Set

Image not found
Thioacetamide
Measured: 6.03
Predicted: 6.43

Image not found
Methyl isothiocyanate
Measured: 9.33
Predicted: 7.63

Image not found
Acetic acid
Measured: 1.00
Predicted: 2.40

Image not found
Epichlorohydrin
Measured: 10.0
Predicted: 9.87

Image not found
Pyridine
Measured: 39.8
Predicted: 20.1